A method for investigating radiation damage

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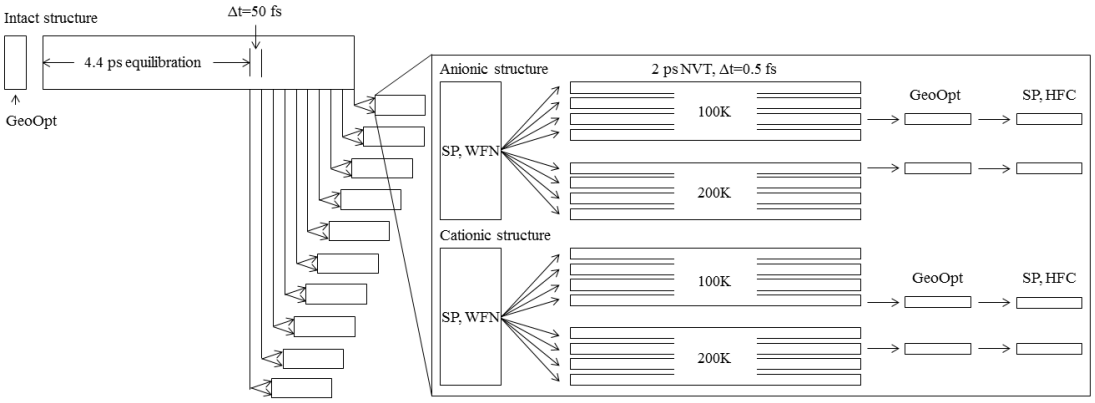
Radiation damaged molecules often have chemical structures significantly different from their undamaged counterparts. The characterization and description of such structures are commonly biased by the investigators experience and imagination. To date, there exist experimental data for which the corresponding chemical structures are unknown. A computational protocol for unbiased generation of possible molecular damages induced by ionizing radiation is needed in order to find such structures and has been devised. The method samples different molecular conformations using *ab initio* molecular dynamics (MD) simulations before the system is ionized and allowed to develop further in time.



In this work, a case study on the carbohydrate α-*l*-rhamnose comprising of 160 *ab initio* MD runs demonstrates 12 different possible radiation damage products. 7 of these potential products have not previously been discussed by either experimentalists or theoreticians. The method suggested in the present work also nicely reproduces other experimentally observed radical structures that previously have been characterized by Electron Magnetic Resonance investigations after irradiation and DFT investigations.

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